Article

Supplementary materials for Stress and Strain Prediction of Zirconium Nitride under Oxygen Doping and Vacancy Introduction

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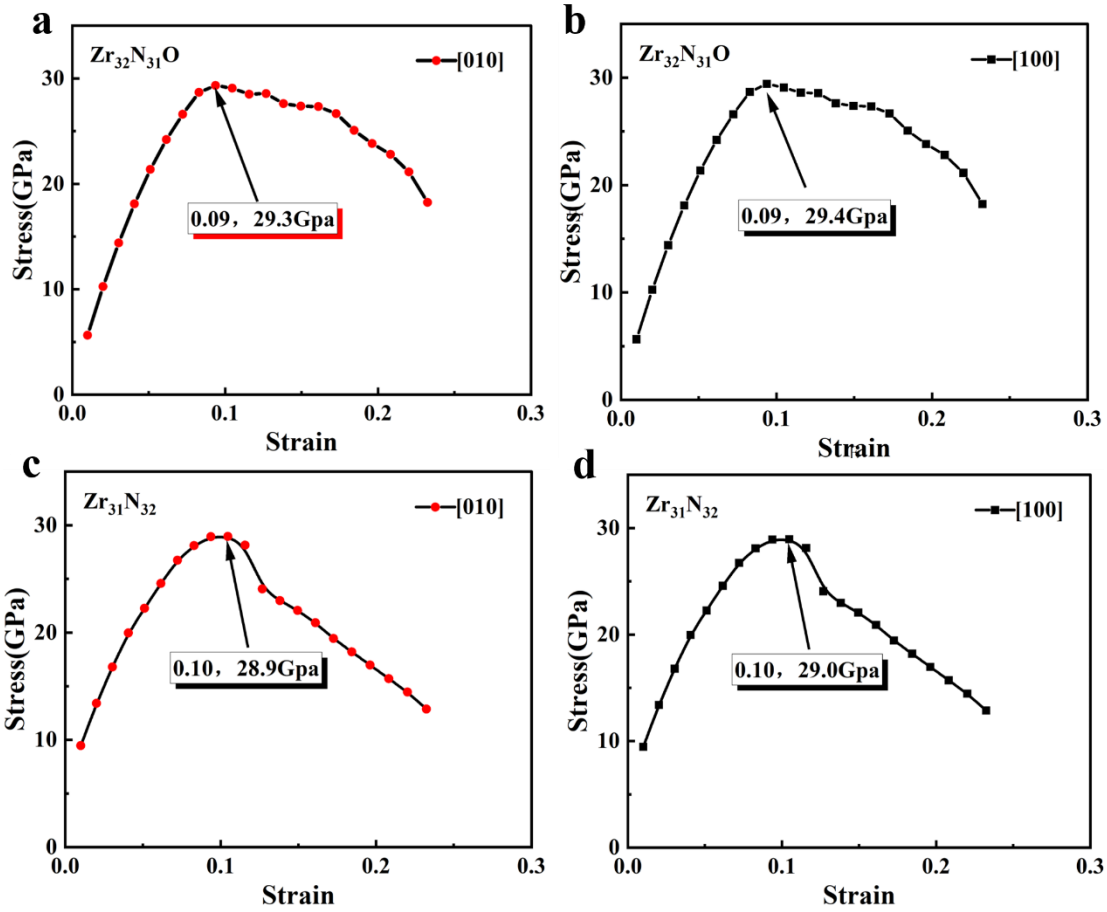

Figure S1. (a) Stress-strain relationship of $Zr_{32}N_{31}O$ in the <010> crystallographic direction. (b) Stress-strain relationship of $Zr_{32}N_{31}O$ in the <100> crystallographic direction. (c) Stress-strain relationship of Zr31N32 in the <010> crystallographic direction. (d) Stress-strain relationship of Zr31N32 in the <100> crystallographic direction.

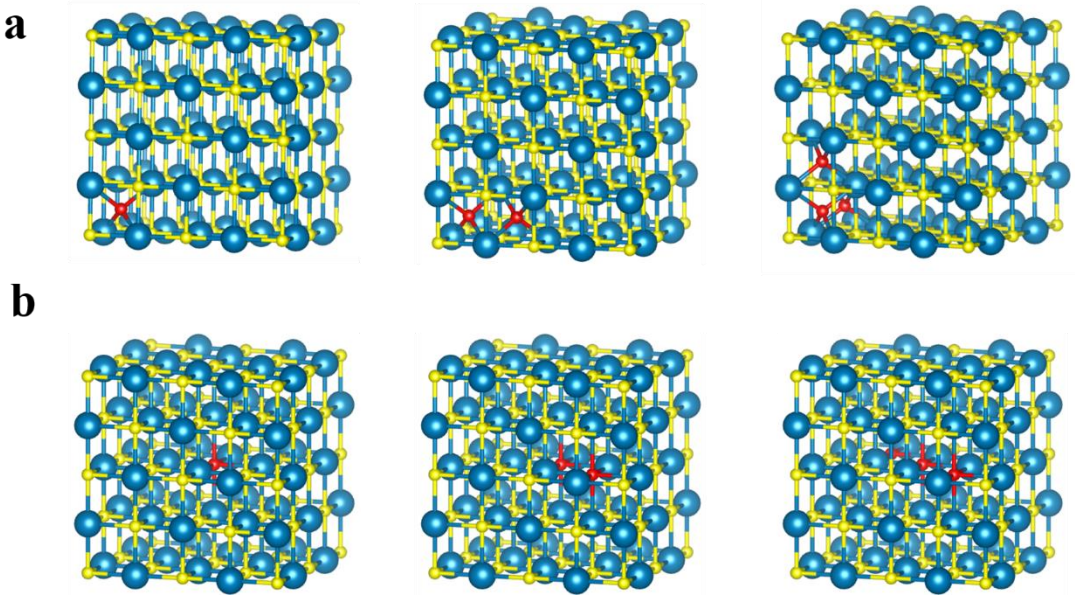

Figure S2. The location of the oxygen atoms during the calculation of formation energy. (a) interstitial oxygen atoms (b) substitutional oxygen atoms.

Table S1. The total energies in the calculation of the formation energy.

Configuration	Energy(eV)	Configuration	Energy(eV)
$E_{Zr_{32}N_{32}O}$	-657.167	$E_{Zr_{32}N_{31}O}$	-649.936
$E_{Zr_{32}N_{32}O_2}$	-662.515	$E_{Zr_{32}N_{30}O_2}$	-647.858
$E_{Zr_{32}N_{32}O_3}$	-666.963	$E_{Zr_{32}N_{29}O_3}$	-645.932